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Quantification of uncertainties in turbulence modeling: A comparison of physics-based and random matrix theoretic approaches

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ABSTRACT

Numerical models based on Reynolds-Averaged Navier-Stokes (RANS) equations are widely used in engineering turbulence modeling. However, the RANS predictions have large model-form uncertainties for many complex flows, e.g., those with non-parallel shear layers or strong mean flow curvature. Quantification of these large uncertainties originating from the modeled Reynolds stresses has attracted attention in the turbulence modeling community. Recently, a physics-based Bayesian framework for quantifying model-form uncertainties has been proposed with successful applications to several flows. Nonetheless, how to specify proper priors without introducing unwarranted, artificial information remains challenging to the current form of the physics-based approach. Another recently proposed method based on random matrix theory provides the prior distributions with maximum entropy, which is an alternative for model-form uncertainty quantification in RANS simulations. This method has better mathematical rigorousness and provides the most non-committal prior distributions without introducing artificial constraints. On the other hand, the physics-based approach has the advantages of being more flexible to incorporate available physical insights. In this work, we compare and discuss the advantages and disadvantages of the two approaches on model-form uncertainty quantification. In addition, we utilize the random matrix theoretic approach to assess and possibly improve the specification of priors used in the physics-based approach. The comparison is conducted through a test case using a canonical flow, the flow past periodic hills. The numerical results show that, to achieve maximum entropy in the prior of Reynolds stresses, the perturbations of shape parameters in Barycentric coordinates are normally distributed. Moreover, the perturbations of the turbulence kinetic energy should conform to log-normal distributions. Finally, the result sheds light on how large the variance of each physical variable should be compared with each other to achieve the approximate maximum entropy prior. The conclusion can be used as a guidance for specifying proper priors in the physics-based, Bayesian uncertainty quantification framework.

Notations

We summarize the convention of notations below because of the large number of symbols used in this paper. The general conventions are as follows:

1. Upper case letters with brackets (e.g., $[R]$) indicate matrices or tensors; lower case letters with arrows (e.g., $\vec{v}$) indicate vectors; undecorated letters in either upper or lower cases indicate scalars. An exception is the spatial coordinate, which is denoted as x for simplicity but is in fact a 3×1 vector. Tensors (matrices) and vectors are also indicated with index notations, e.g., R_{ij} and v_i with $i, j = 1, 2, 3$.
2. Bold letters (e.g., $[\mathbf{R}]$) indicate random variables (including scalars, vectors, and matrices), the non-bold letters (e.g., $[R]$) indicate the corresponding realizations, and underlined letters (e.g., $[\,\underline{R}\,]$) indicate the mean.
3. Symbols $\mathbb{M}_d^+$, and $\mathbb{M}_d^{+0}$ indicate the sets of symmetric positive definite and symmetric positive semi-definite matrices, respectively, of dimension $d \times d$ with the following relation: $\mathbb{M}_d^+ \subset \mathbb{M}_d^{+0} \subset \mathbb{M}_d^s$.

This work deals with Reynolds stresses, which are rank two tensors. Therefore, it is implied throughout the paper that all random or deterministic matrices have sizes 3×3 with real entries unless noted otherwise. Finally, a list of nomenclature is presented in Appendix C.

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1. Introduction

Despite the increasing availability of computational resources in the past decades, high-fidelity simulations (e.g., large eddy simulation, direct numerical simulation) are still not affordable for most practical problems. Numerical models based on Reynolds-Averaged Navier–Stokes (RANS) equations are still the dominant tools for the prediction of turbulent flows in industrial and natural processes. However, for many practical flows, e.g., those with strong adverse pressure gradient, non-parallel shear layers, or strong mean flow curvature, the predictions of RANS models have large uncertainties. The uncertainties are mostly attributed to the phenomenological closure models for the Reynolds stresses (Oliver and Moser, 2009; Pope, 2000). Previous efforts in quantifying and reducing model-form uncertainties in RANS simulations have mostly followed parametric approaches, e.g., by perturbing, tuning, or inferring the parameters of the closure models of the Reynolds stress (Edeling et al., 2014a; 2014b; Margheri et al., 2014).

Recently, the turbulence modeling community has recognized the limitations of the parametric approaches and started investigating non-parametric approaches where uncertainties are directly injected into the Reynolds stresses (Dow and Wang, 2011; Emory et al., 2013; 2011; Gorlé and Iaccarino, 2013; Oliver and Moser, 2009; Xiao et al., 2015). In their pioneering work, Iaccarino et al. (Emory et al., 2013; 2011; Gorlé and Iaccarino, 2013) proposed a physics-based approach, where the Reynolds stress is projected onto six physically meaningful dimensions (its shape, magnitude, and orientation). They further perturbed the Reynolds stresses towards the limiting states in the physically realizable range, based on which the RANS prediction uncertainties are estimated. Building on the work of Iaccarino et al. (Emory et al., 2013; 2011; Gorlé and Iaccarino, 2013), Xiao et al. (2015) modeled the Reynolds stress discrepancy as a *zero-mean random field* and used a physical-based parameterization to systematically explore the uncertainty space. They further used Bayesian inferences to incorporate observation data to reduce the model-form uncertainty in RANS simulation. While the physics-based method has achieved significant successes, the method in its current form has two major limitations. First, uncertainties are only injected to the shape and magnitude of the Reynolds stresses but not to the orientations, and thus they do not fully explore the uncertainty space. Second, it is challenging to specify prior distributions over these physical variables without introducing artificial constraints. The priors are critical for uncertainty propagation and Bayesian inference, particularly when the amount of data is limited (Wang et al., 2015). Xiao et al. (2015) specified Gaussian distribution for the perturbations of shape parameters in natural coordinates and log-normal distribution for the turbulence kinetic energy discrepancy. The perturbations in all physical parameters share the same variance field. However, it is not clear if or how much artificial constraints are introduced into the prior with this choice. Moreover, without sufficient physical insight, it is not clear how large the variance of perturbation for each physical variable should be relative to each other.

In information theory, Shannon entropy is an important measure of the information contained in each probability distribution. The distribution best representing the current state is the one with the largest information entropy, which is known as principle of maximum entropy (Guiasu and Shenitzer, 1985). This principle has been used as a guideline to specify prior distributions in Bayesian framework (Jaynes, 1957). Although this theory has been extensively used in information processing problems such as communications and image processing, the application in conjunction with random matrix theory applied to physical systems is only a recent development, which was first proposed and developed by Soize (2000) and Das and Ghanem (2009). Built on the theories developed by Soize et al., Xiao and Ghanem (2016) proposed a random matrix theoretic (RMT) approach with maximum entropy principle to quantify model-form uncertainties in RANS simulations. The RMT approach is an alternative to the physics-based approach in quantifying model-form uncertainties in RANS simulations. In this approach, the realizability of perturbed Reynolds stresses is guaranteed automatically in a mathematical way, since the uncertainties are directly injected within the set $\mathbb{M}_d^{+0}$ of positive semidefinite matrices. In addition, the RMT approach can provide objective priors for Bayesian inferences that satisfy the given constraints without introducing artificial information.

While the RMT approach has better mathematical rigorousness and provides a proper prior of the Reynolds stress tensors with maximum entropy, it has its own limitations. In particular, since the perturbations are directly introduced to the Reynolds stress itself, it is not straightforward to incorporate physical insights that are available for specific flows into the RMT approach. For example, for the flow in a channel with square cross section, the discrepancies of RANS-predicted Reynolds stress mainly come from the shape of the Reynolds stress tensor, while the predicted turbulence kinetic energy is rather accurate (Wu et al., 2015). In this case, the perturbation variances of shape parameters should be specified much larger than that of the turbulence kinetic energy. Nonetheless, this piece of information is difficult to incorporate into the RMT approach. In comparison, the physics-based approach is more flexible and thus may be preferred in engineering applications for both uncertainty quantification and Bayesian inferences. The objective of this work is twofold. First, we compare the physics-based approach and RMT approach on model-form uncertainty quantification and propagation. The advantages and disadvantages of both approaches are discussed. Second, we use the results from the RMT approach to assess the artificial constraints introduced in the physics-based approach and possibly improve the specification of physics-based priors under the context of Bayesian inference. To this end, the Reynolds stress samples with maximum entropy distribution obtained in the RMT approach are first projected onto the physically meaningful dimensions. Then, the distributions in the six physical dimensions are used to compare with the priors specified in the physics-based approach. The perturbed Reynolds stresses from both approaches are propagated to the quantities of interest (QoIs), e.g., velocity field and wall shear stress, and the differences of these propagated QoIs are investigated. The comparisons can provide useful insights on the model-from uncertainty quantification in RANS modeling. Moreover, they also sheds light on the specification of appropriate prior for each physical variable when no further physical knowledge is available.

This work is the first attempt to fully explore the uncertainty space in physics-based approach. The orientations of Reynolds stresses are perturbed, and their impacts on the propagated QoIs are investigated. Note that in this work we only focus on uncertainty propagation (i.e., prior). The assessment of posterior from Bayesian inference is not included. This is because the inversion schemes currently used for reducing RANS model-form uncertainties are approximate Bayesian approaches, e.g., iterative ensemble Kalman filtering in Wang et al. (2015) and Xiao et al. (2015), which are not sensitive to the prior and cannot provide a posterior uncertainty estimation with a comparable accuracy to that obtained from the exact Bayesian sampling scheme (Law and Stuart, 2012). This compromise is under the consideration of high computational costs of RANS model evaluations, which make exact Bayesian approach (i.e., Markov Chain Monte Carlo (MCMC) sampling scheme) prohibitively expensive. Obtaining an accurate posterior is still an ongoing work, which can be possibly achieved by utilizing recently developed dimension reduction methods (e.g., active subspace methods Constantine et al., 2015) and fast sampling